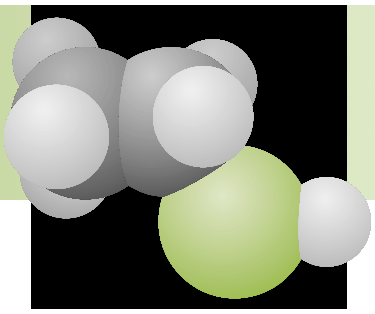
CHEMICALS

Project Fact Sheet



COMPUTATIONAL CHEMISTRY AND REACTION ENGINEERING WORKBENCH

BENEFITS

- Increases energy savings due to increased process efficiency
- Decreases emissions
- Increases product yield

APPLICATIONS

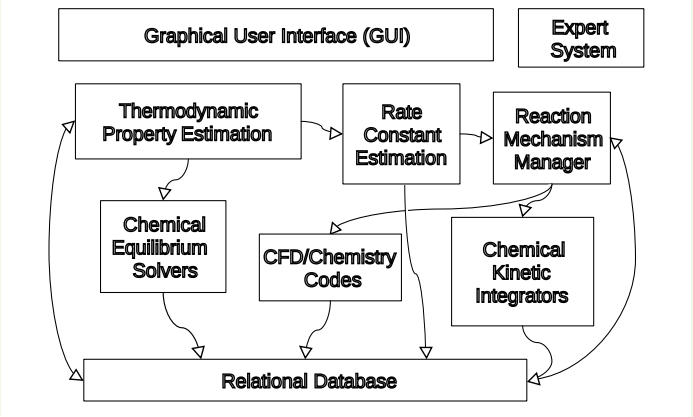
CCRE Workbench will be used in the design and optimization of pyrolysis reactors, boilers and furnaces, and atmospheric reactions. Optimization of the combustion process in boilers and furnaces could lead to energy savings in many industries including chemicals, petroleum, forest products, steel, mining, and aluminum.

INTEGRATION OF COMPUTATIONAL TOOLS WILL IMPROVE PROCESS EFFICIENCIES

To meet the challenges of the 21st century, the U.S. chemical industry will increasingly rely on modeling to improve efficiencies, enhance product quality, lower energy consumption, and reduce unwanted emissions. Currently, a broad array of computational chemistry tools exists. However, the learning curve required to implement these tools is so steep that their use has been limited. This project will develop new software that will integrate a suite of computational chemistry tools into a unified package, with a graphical, user-friendly interface.

The project is focusing on integrating computational chemistry models into a unified problem-solving environment, titled *Computational Chemistry and Reaction Engineering (CCRE) Workbench*. The *CCRE Workbench* will include several components: thermodynamic property estimation, rate constant estimation methods, chemical kinetic integrators, reaction mechanism manager, equilibrium solver, sensitivity and error analysis, optimization and parameter estimation, and mechanism reduction. While software exists for most of these components, there are no standards for input and output data formats, conventions, or philosophy for obtaining results. The graphical, user-friendly interface, and on-line expert help system offered by this package will result in a significantly reduced learning curve and increased implemenation by plant process engineers.

LOGIC CHART



Schematic diagram of the high-level components of the CCRE Workbench and their major interconnections.

Project Description

Goal: Develop an integrated computational chemistry program that will benefit both specialists and process engineers.

Progress and Milestones

This project is divided into the following activities:

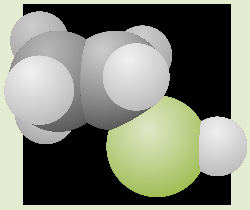
CCRE Workbench Computational Chemistry Components
- Thermodynamic Property Estimation
- Rate Constant Estimation Methods
- Chemical Kinetic Integrators
- Reaction Mechanism Manager
- Equilibrium Solver
- Sensitivity and Error Analysis
- Optimization and Parameter Estimation
- Mechanism Reduction
- Remote/Distributed Database

CCRE Workbench Operational Components
- Graphical User Interface
- Distributed Computing
- Data Visualization
- Local Relational Database
- Expert System
- Report Generation

Development of Educational Modules
- Chemical Reaction Engineering
- Combustion Chemistry
- Atmospheric Chemistry
- Physical Chemistry

Commercialization

Reaction Design, Inc. will be responsible for the commercial evaluation and potential implementation of the *CCRE Workbench* system. They have experience in sales and marketing in the chemical industry. Additionally, Reaction Design has commercialized software to aid in the design of chemical reaction processes. After successful trials of the initial *CCRE Workbench* prototype, Reaction Design will produce and market a commercial software product to the academic, National Laboratory, and industrial research and design communities.



Project Partners

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National Renewable Energy Laboratory
Golden, CO

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Annandale, NJ

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